



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 10:37 pm BST

PDB ID : 1A3Q  
Title : HUMAN NF-KAPPA-B P52 BOUND TO DNA  
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Deposited on : 1998-01-23  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

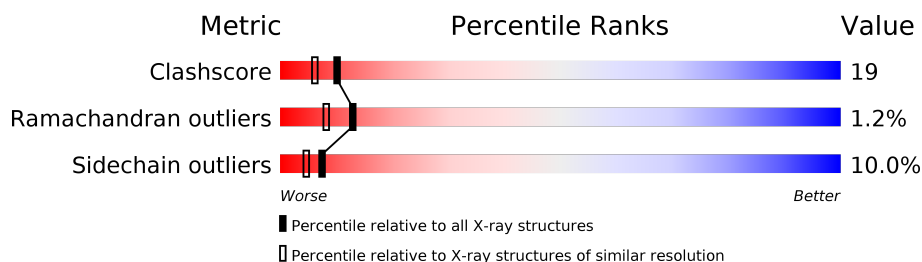
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	11	<div> <div>91%</div> <div>9%</div> </div>
2	D	11	<div> <div>45%</div> <div>55%</div> </div>
3	A	285	<div> <div>60%</div> <div>36%</div> <div>.</div> </div>
3	B	285	<div> <div>57%</div> <div>37%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5748 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(\*GP\*GP\*GP\*GP\*AP\*AP\*TP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	P	0	0	0
			222	106	41	65	10			

- Molecule 3 is a protein called PROTEIN (NUCLEAR FACTOR KAPPA-B P52).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	285	Total	C	N	O	S	0	0	0
			2259	1423	409	415	12			
3	B	285	Total	C	N	O	S	0	0	0
			2259	1423	409	415	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ILE	THR	CONFLICT	UNP Q00653
B	213	ILE	THR	CONFLICT	UNP Q00653

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	32	Total	O	0	0
			32	32		
4	D	41	Total	O	0	0
			41	41		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	377	Total 377	O 377	0	0
4	B	335	Total 335	O 335	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*GP\*GP\*GP\*GP\*AP\*AP\*TP\*CP\*CP\*CP\*C)-3')

Chain C: 



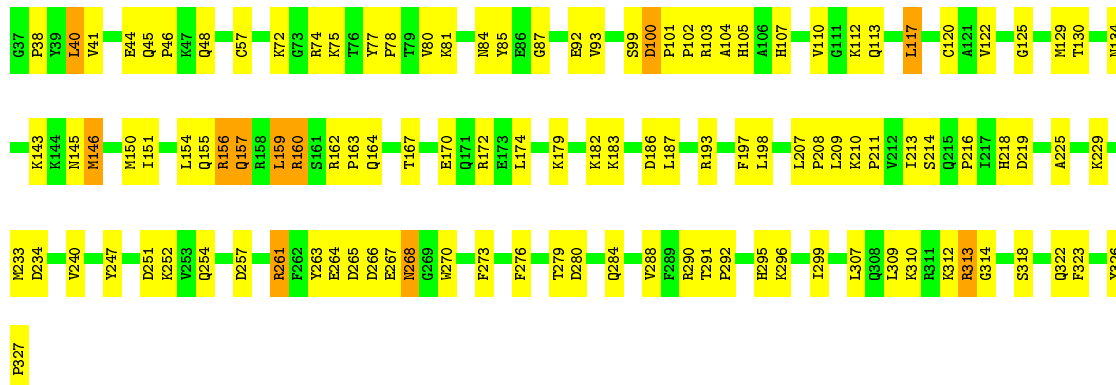
- Molecule 2: DNA (5'-D(\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*CP\*CP\*CP\*C)-3')

Chain D: 



- Molecule 3: PROTEIN (NUCLEAR FACTOR KAPPA-B P52)

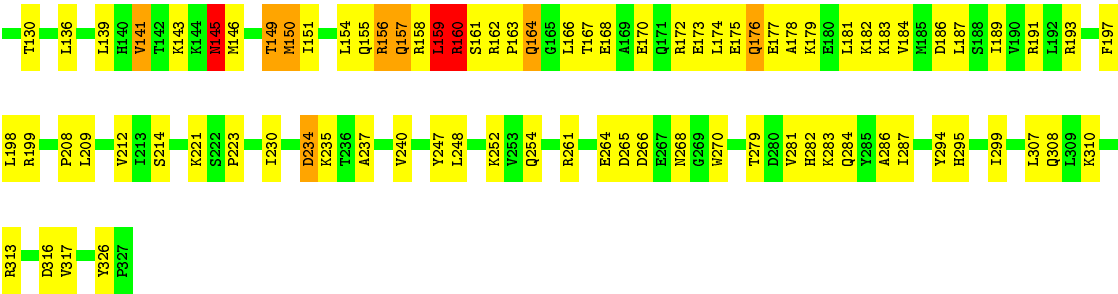
Chain A: 



- Molecule 3: PROTEIN (NUCLEAR FACTOR KAPPA-B P52)

Chain B: 





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.20 Å   121.00 Å   134.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.8 (10.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	6.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.219 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.86	0/250	1.04	0/384
2	D	0.89	0/248	1.13	2/381 (0.5%)
3	A	0.60	0/2307	0.89	2/3104 (0.1%)
3	B	0.63	0/2307	0.91	6/3104 (0.2%)
All	All	0.65	0/5112	0.92	10/6973 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
3	A	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	GLN	N-CA-C	7.45	131.12	111.00
3	B	117	LEU	CB-CG-CD1	-7.38	98.46	111.00
3	B	164	GLN	N-CA-C	6.82	129.42	111.00
3	A	117	LEU	CB-CG-CD1	-6.44	100.05	111.00
2	D	605	DG	O5'-C5'-C4'	5.79	125.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	263	TYR	Sidechain
2	D	614	DC	Sidechain



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	223	0	124	2	0
2	D	222	0	125	3	0
3	A	2259	0	2279	87	0
3	B	2259	0	2279	95	0
4	A	377	0	0	12	0
4	B	335	0	0	8	0
4	C	32	0	0	0	0
4	D	41	0	0	2	0
All	All	5748	0	4807	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 185 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:117:LEU:HD11	3:B:156:ARG:HD2	1.14	1.14
3:B:117:LEU:CD1	3:B:156:ARG:HD2	2.04	0.84
3:A:102:PRO:HG3	3:A:213:ILE:HD11	1.62	0.82
3:A:218:HIS:HB3	3:A:225:ALA:HB1	1.60	0.82
3:A:162:ARG:HB3	3:A:163:PRO:HD2	1.63	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	281/285 (99%)	250 (89%)	29 (10%)	2 (1%)	22	18
3	B	281/285 (99%)	252 (90%)	24 (8%)	5 (2%)	8	4
All	All	562/570 (99%)	502 (89%)	53 (9%)	7 (1%)	13	8

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	87	GLY
3	B	125	GLY
3	A	125	GLY
3	B	116	GLU
3	B	145	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	249/249 (100%)	226 (91%)	23 (9%)	9	6
3	B	249/249 (100%)	222 (89%)	27 (11%)	6	3
All	All	498/498 (100%)	448 (90%)	50 (10%)	7	5

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	313	ARG
3	B	103	ARG
3	B	268	ASN
3	B	72	LYS
3	B	79	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	322	GLN

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Mol	Chain	Res	Type
3	B	84	ASN
3	B	157	GLN
3	A	295	HIS
3	B	176	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	1
3	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	199:ARG	C	206:SER	N	6.86
1	B	199:ARG	C	206:SER	N	6.82

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.